To: Volz, Stephanie[Volz.Stephanie@epa.gov]
From: Strynar, Mark[/O=EXCHANGELABS/OU=EXCHANGE ADMINISTRATIVE GROUP (FYDIBOHF23SPDLT)/CN=RECIPIENTS/CN=5A9910D5B38E471497BD875FD329A20A-STRYNAR, MARK]
Sent: Wed 8/28/2019 8:02:29 PM (UTC)
Subject: RE: PFAS Question
strynar et al., 2015 SI.pdf
Strynar et al., 2015 ES&T.pdf

Stephanie,

First for the PFESA BP2, yes having two peaks is typical. Something about having asymmetric carbons or something like that. I don't recall the details. The peaks are usually exactly the same size, but for sure 2 peaks.

For the PFESA BP1 and the PFO5DoDA they are similar in molecular weight however two things will stand out.

1. The molecular weight between two compounds PFESA BP1 (442.9264) and PFO5DoDA (442.9442) is 40.2 ppm. Your QTOF should be able to tell them apart based on mass due to the EIC being extracted can be chosen to be +/- 5 ppm or so.
2. The PFESA BP1 will have a sulfonate (m/z 79.9) and a FSO3 (m/z 98.9) transition just like the PFOS, PFHxS and PFBS do.
3. PFO5DoDA will have a 84.9907 fragment however the PFESA BP1 will not. I have no idea what the 283.1367 fragment is. Also it will

Glad to chat if you need more later on tomorrow. Here is my 2015 paper in the SI that may have some details you can use. I also have standards for all of these I can share if you need them.

Mark

From: Volz, Stephanie <Volz.Stephanie@epa.gov>
Sent: Wednesday, August 28, 2019 3:06 PM
To: Strynar, Mark <Strynar.Mark@epa.gov>
Subject: PFAS Question

Mark,
I just left you a phone message but was wondering if you have any insight or documentation into telling these two compounds (PFESA Byproduct 1 and PFO5DA) apart. I don't have any reference material but I am working on a QTOF. I'm seeing 442.943 and 886.896 for the dimer. I'm seeing the peak at 8.175 minutes and fragments of 283.1367 and 84.9907. I don't have background data on retention time or fragments for either compound.

Compound Name	Formula	RT (min)	Mass	m/z	Adduct/dimer	Frag
PFESA (Byproduct 1)	C7HF13O5S		443.93371	442.9441926	886.8596 (2M-H)-	
PFO5DA	C7HF13O7		443.95147	442.926434	886.8951 (2M-H)-	

Also, I'm seeing a doublet for PFESA Byproduct 2 at 7.171 and 7.294 minutes. Do you know if that's typical?

Best Regards,

Stephanie Volz
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